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FILE COVERS 1907 - 31 Mar 2003  VOL 138 ISS 14
FILE LAST UPDATED: 30 Mar 2003  (20030330/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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=> d stat que l8
L3              STR
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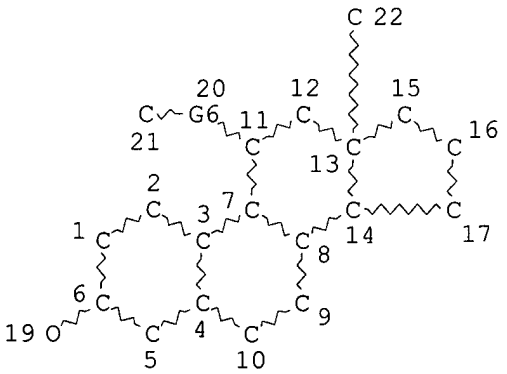


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  21

STEREO ATTRIBUTES: NONE
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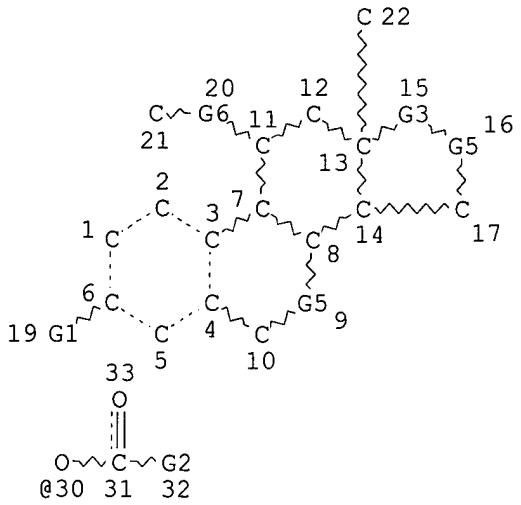
antecedent

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HO~CH 25 @26

HO~C~G4 27 @28 29

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VAR G3=26/28
VAR G4=AK/CY
VAR G5=CH2/23
REP G6=(4-8) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE
L7 115 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
L8 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

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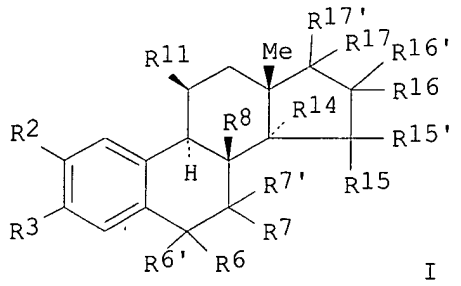
=> d ibib abs hitrn 18 1-12

L8 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:763026 HCAPLUS
DOCUMENT NUMBER: 135:318607
TITLE: Preparation of 8.beta.-substituted-11.beta.-pentyl- and 11.beta.-hexyl-estra-1,3,5(10)-triene derivatives which have an affinity for the estrogen receptor
INVENTOR(S): Peters, Olaf; Braeuer, Nico; Hillisch, Alexander; Hegele-Hartung, Christa; Fritzemeier, Karl-Heinrich
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|

WO 2001077138 A1 20011018 WO 2001-EP4289 20010412
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
DE 10019167 A1 20011018 DE 2000-10019167 20000412
EP 1272505 A1 20030108 EP 2001-940331 20010412
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
NO 2002004907 A 20021205 NO 2002-4907 20021011
PRIORITY APPLN. INFO.: DE 2000-10019167 A 20000412
US 2000-207370P P 20000526
WO 2001-EP4289 W 20010412
OTHER SOURCE(S): MARPAT 135:318607
GI

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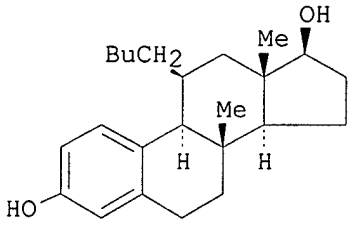
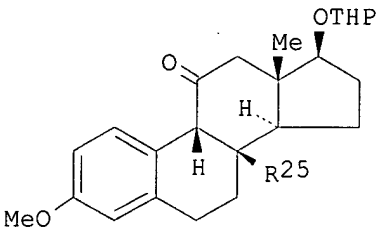



II




III

AB The present invention relates to the novel 8.beta.-substituted estra-1,3,5(10)-trienes I [R2 = H, F, Cl, Br, I, straight or branched (un)satd. C1-6-alkyl, OH, alkoxy, acyloxy, CF3, sulfamoyloxy; R3 = alkoxy, sulfamoyloxy, acyloxy; R6, R6' = H; R6R7 = bond; R7, R7' = H ; R8 means a straight-chain or branched-chain, optionally partially or entirely halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an ethynyl or prop-1-inyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 = bond ; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy, acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8.beta.-methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol (II) was prepd. from 8.beta.-cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher

affinity of estrogen receptor prepns. of rat prostate than of estrogen receptor prepns. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the prodn. thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

IT **367269-66-7P**, 8.beta.-Methyl-11.beta.-pentylestra-1,3,5(10)-triene-3,17.beta.-diol **367269-67-8P**, 11.beta.-Hexyl-8.beta.-methylestra-1,3,5(10)-triene-3,17.beta.-diol **367269-79-2P**, 11.beta.-Pentyl-8.beta.-vinylestra-1,3,5(10)-triene-3,17.beta.-diol **367269-80-5P**, 11.beta.-Hexyl-8.beta.-vinylestra-1,3,5(10)-triene-3,17.beta.-diol **367269-81-6P**, 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol **367269-82-7P**, 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol **367269-89-4P**, 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate **367269-90-7P**, 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate **367269-91-8P**, 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate **367269-92-9P**, 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate **367269-93-0P**, 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate **367269-94-1P**, 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 8.beta.-substituted-11.beta.-pentyl- and -11.beta.-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the estrogen receptor)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:435020 HCAPLUS
DOCUMENT NUMBER: 135:19815
TITLE: Preparation of anti-estrogen compounds having hydroxycarbonyl-halogenoalkyl side chain
INVENTOR(S): Jo, Jaechon; Kwon, Heean; Lim, Hyunsuk; Choi, Jaeyoung; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myunghwa; Nishimura, Yoshikazu
PATENT ASSIGNEE(S): C + C Research Laboratories, S. Korea
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001042186 | A1 | 20010614 | WO 2000-JP8810 | 20001213 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | | |
|---|---|---|---|---|---|
| AU 2001018883 | A5 | 20010618 | AU 2001-18883 | 20001213 | |
| EP 1241158 | A1 | 20020918 | EP 2000-981681 | 20001213 | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | | |
| JP 3357356 | B2 | 20021216 | JP 2001-54388 | 20001213 | |
| JP 2003040834 | A2 | 20030213 | JP 2002-199200 | 20001213 | |
| NO 2002002783 | A | 20020813 | NO 2002-2783 | 20020611 | |

PRIORITY APPLN. INFO.:
JP 1999-353640 A 19991213
JP 2000-100567 A 20000403
JP 2000-186684 A 20000621
JP 2000-232091 A 20000731
JP 2000-357793 A 20001124
JP 2001-543488 A3 20001213
WO 2000-JP8810 W 20001213

OTHER SOURCE(S): MARPAT 135:19815
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. in which either a compd. having reduced oral activity or a group having a framework thereof is chem. bonded to a group represented by the general formula (CH2)mCH(CO2R1)(CH2)nR2 (wherein R1 represents hydrogen, metal forming a salt; R2 represents linear or branched C1-7 halogenoalkyl; m is an integer of 2 to 14; and n is an integer of 2 to 7), optical isomers of the compds.; or hydrates or pharmacol. acceptable salts of these compds. are prepd. When imparted to a framework of, e.g., estradiol Q or Q1, 2-(p-hydroxyphenyl)-6-naphthol Q2, or 2-(4-hydroxyphenyl)-2-(4-hydroxybenzoyl)-6-hydroxybenzo[b]thiophene Q3, etc., a compd. having anti-estrogen activity, those compds. represented by formula A-(CH2)mCH(CO2R1)(CH2)nR2 (A = Q, Q1, Q2, Q3, etc.), a compd. having anti-estrogen activity, those can have significantly improved oral activity. The compds. are hence useful as antitumor agents, in particular for the treatment of breast cancer. Thus, cross-metathesis of 3-methoxy-7.alpha.-(2-propenyl)estra-1,3,5(10)-trien-17.beta.-ol with (4R,5S)-3,4-dimethyl-1-[(2S)-2-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-8-nonenoyl]-5-phenylimidazolidin-2-one in the presence of Grubbs' catalyst followed by hydrogenation oxidative hydrolysis, and demethylation gave (2S)-10-(3,17.beta.-dihydroxyestra-1,3,5(10)-trien-7.alpha.-yl)-2-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)decanoic acid (I). I at 10 mg/kg p.o. per day for 3 days inhibited by 100% the 17.beta.-estradiol benzoate-stimulated increase in the uterus wt. in mice.

IT **342898-68-4P 342898-92-4P 342898-96-8P**
**342898-97-9P 342898-98-0P 342898-99-1P**
**342899-00-7P 342899-25-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of anti-estrogen compds. having hydroxycarbonyl-haloalkyl side chain as antitumor agents for treatment of breast cancer with improved oral activity)

IT **342898-67-3P 342898-91-3P 342899-24-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of anti-estrogen compds. having hydroxycarbonyl-haloalkyl side chain as antitumor agents for treatment of breast cancer with improved oral activity)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:190285 HCAPLUS
DOCUMENT NUMBER: 134:261332
TITLE: QSAR with electrotopological state atom index. Part-3a. Receptor binding affinity of estrogens and non-steroidal estrogen analogs
AUTHOR(S): Saha, Achintya; Roy, Kunal; De, Kakali; Sengupta, Chandana
CORPORATE SOURCE: Dep. Chemical Technology, Univ. Calcutta, alcutta, 700 009, India
SOURCE: Journal of the Indian Chemical Society (2001), 78(2), 92-97
CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER: Indian Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Quant. structure activity relationship (QSAR) anal. of estrogens and non-steroidal analogs of estrogen with electrotopol. state atom (ETSA) index has been performed to explore the atoms or fragments of the mols. that are most important for the binding affinity to receptor. The study reveals the importance of Ph ring fragment (C1, C5 and C10 atoms of steroidal estrogen, and C1, C3, C4, C9 and C10 atoms in case of non-steroidal analogs) for receptor binding affinity. The importance of these atoms or fragments is also supported from the literature survey. Thus, the Ph ring constitutes the pharmacophore for receptor binding affinity of estrogen analogs. Hence, diagnostic potential of the ETSA scheme in identifying the atoms or fragments important for activity is revealed from the study.

IT **134411-55-5 134411-57-7**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(QSAR with electrotopol. state atom index in relation to receptor binding affinity of estrogens and non-steroidal estrogen analogs)

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:909685 HCAPLUS
DOCUMENT NUMBER: 134:56837
TITLE: Methods for the production of long-chain substituted estratriene and their application in the preparation of medicaments
INVENTOR(S): Sauer, Gerhard; Bohlmann, Rolf; Heinrich, Nikolaus; Kroll, Jorg; Zorn, Ludwig; Fritzmeier, Karl-Heinrich; Hegele-Hartung, Christa; Hoffmann, Jens; Lichtner, Rosemarie
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 19929715 | A1 | 20001228 | DE 1999-19929715 | 19990624 |
| WO 2001000652 | A2 | 20010104 | WO 2000-EP5969 | 20000626 |
| WO 2001000652 | A3 | 20010510 | | |

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,

SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ,
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
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CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
AU 2000061524 A5 20010131 AU 2000-61524 20000626
EP 1187846 A2 20020320 EP 2000-947882 20000626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO
JP 2003503419 T2 20030128 JP 2001-507059 20000626
NO 2001006330 A 20020131 NO 2001-6330 20011221
PRIORITY APPLN. INFO.: DE 1999-19929715 A 19990624
WO 2000-EP5969 W 20000626
OTHER SOURCE(S): MARPAT 134:56837
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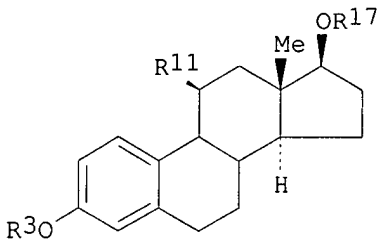


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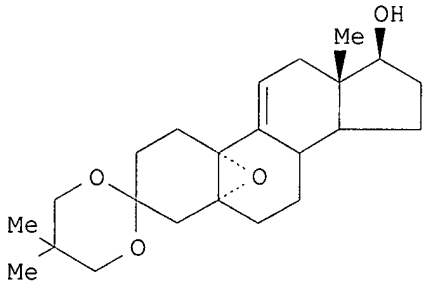



II

AB This invention describes the synthesis of new antiesterogenic 11.beta. long-chain substituted estratriene [I; R3 = H, alkyl, R3'C(O); R3' = H, alkyl, ph; R11 = ABZR20; A = bond, phenylene, phenyleneoxy; B = alkylene, alkenylene, alkynylene; Z = NR21; R21 = alkyl; R20 = H, alkyl, alkenyl, -alkynyl, DCnFn+1; D = aryl, alkylene, alkenylene, alkynylene; n = 1 - 8; R20 = LCH=CFCpF2p+1; L = alkylene, alkenylene, alkynylene; p = 2-7; R20 = DO(CH2)q-aryl; q = 0 - 3; aryl = Ph, 1-naphthyl, 2-naphthyl, heteroaryl; DO(CH2)rCnF2n+1; r = 1 - 5; R20R21 with N = C5-C6-heterocycle; R20R21 with N = heterocycle etc.; R17 = H, R17'C(O); R17' = H, alkyl] for the prodn. of medicaments. Thus, I [R3, R17 = H; R11 = F5C2(CH2)3S(CH2)3N(Me)(CH2)5] was prepd. from epoxyestrene (II) via reaction with 1-bromo-5-tert-butyldimethylsilyloxypentane, aromatization, chlorination and amination with methyl{3-[(4,4,5,5,5,5-pentafluoropentyl)sulfanyl]propyl}amine. Formulations of I (no data) are claimed.

IT **314019-28-8P 314019-30-2P 314019-32-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of long-chain substituted estratriene and their application in the prepn. of medicaments)

IT **151555-65-6P 314019-26-6P 314019-27-7P**
**314019-29-9P 314019-31-3P 314019-33-5P**
**314019-58-4P 314019-59-5P 314019-60-8P**
**314019-61-9P 314019-62-0P 314019-63-1P**
**314019-64-2P 314019-65-3P 314019-66-4P**
**314019-67-5P 314019-68-6P 314019-69-7P**
**314019-70-0P 314019-71-1P 314019-72-2P**
**314019-73-3P 314019-74-4P 314019-75-5P**
**314019-76-6P 314019-77-7P 314019-78-8P**
**314019-79-9P 314019-80-2P 314019-81-3P**
**314019-82-4P 314019-83-5P 314019-84-6P**
**314019-85-7P 314019-86-8P 314019-87-9P**

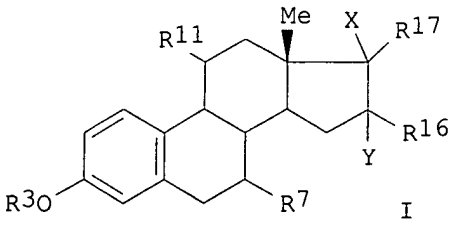
**314019-88-0P 314019-89-1P 314019-90-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of long-chain substituted estratriene and their application in the prepn. of medicaments)

IT **314019-42-6P 314019-43-7P 314019-45-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of long-chain substituted estratriene and their application in the prepn. of medicaments)

L8 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:368399 HCAPLUS
DOCUMENT NUMBER: 133:4848
TITLE: Preparation of estrogenic estra-1,3,5(10)-trienes with differential effects on the .alpha. and .beta. estrogen receptors, having a linear hydrocarbon chain of from 5-9 carbon atoms in position 11
INVENTOR(S): Loozen, Hubert Jan Jozef; Schoonen, Wilhelmus Gerardus Eduardus Joseph
PATENT ASSIGNEE(S): Akzo Nobel N.V., Neth.
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000031112 | A1 | 20000602 | WO 1999-EP9053 | 19991118 |
| W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1131336 | A1 | 20010912 | EP 1999-963327 | 19991118 |
| EP 1131336 | B1 | 20020828 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| AT 222922 | E | 20020915 | AT 1999-963327 | 19991118 |

PRIORITY APPLN. INFO.: EP 1998-203914 A 19981120
WO 1999-EP9053 W 19991118
OTHER SOURCE(S): MARPAT 133:4848
GI



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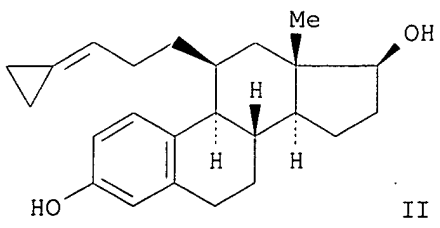


II

AB Novel 11.beta.-substituted estradiols of formula I [R3 = H, acyl, aroyl; R7, R16, R17 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aryl; R11 = linear

or branched hydrocarbon chain; X, Y = H, OH] are prepd. The resulting compds. have a desirable mixed agonist/antagonist profile for estrogen receptor .alpha. and estrogen receptor .beta.. Thus, II was prepd. and was an agonist for ER.alpha. and an antagonist for ER.beta..

IT **271259-96-2P 271260-03-8P 271260-07-2P**
**271260-09-4P 271260-12-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of estrogenic 11-substituted estratrienes with differential effects on estrogen receptors)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:576677 HCAPLUS
DOCUMENT NUMBER: 127:171883
TITLE: Method of treating alopecia
INVENTOR(S): Smart, Robert C.; Oh, Hye-sun
PATENT ASSIGNEE(S): North Carolina State University, USA; Smart, Robert C.; Oh, Hye-Sun
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9730697 | A1 | 19970828 | WO 1997-US2385 | 19970218 |
| W: AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, CZ, DE, DE, DK, DK, EE, EE, ES, FI, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| CA 2247258 | AA | 19970828 | CA 1997-2247258 | 19970218 |
| AU 9720513 | A1 | 19970910 | AU 1997-20513 | 19970218 |
| AU 725243 | B2 | 20001012 | | |
| EP 938296 | A1 | 19990901 | EP 1997-908659 | 19970218 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| JP 2000505454 | T2 | 20000509 | JP 1997-530248 | 19970218 |
| US 6204258 | B1 | 20010320 | US 1999-257396 | 19990225 |

PRIORITY APPLN. INFO.: US 1996-604448 A1 19960221
WO 1997-US2385 W 19970218

OTHER SOURCE(S): MARPAT 127:171883

AB A method of enhancing hair growth or treating alopecia in a subject uses topically administered estrogen receptor antagonists. Within 3 wk, topical application of the estrogen receptor antagonist ICI 182780 (10 nmol, twice weekly) induced full hair regrowth on clipped dorsal skin of 60% of the treated mice, as compared to 40% of the vehicle only treated mice.

IT **134411-55-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(alopecia treatment with estrogen receptor antagonists)

10 carbons

L8 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:435821 HCAPLUS
DOCUMENT NUMBER: 127:76140
TITLE: Steroidal Affinity Labels of the Estrogen Receptor. 3. Estradiol 11.beta.-n-Alkyl Derivatives Bearing a Terminal Electrophilic Group: Antiestrogenic and Cytotoxic Properties
AUTHOR(S): Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; Nique, Francois; Teutsch, Georges; Borgna, Jean-Louis
CORPORATE SOURCE: INSERM Unite 439, Montpellier, 34090, Fr.
SOURCE: Journal of Medicinal Chemistry (1997), 40(14), 2217-2227
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB With the aim of developing a new series of steroidal affinity labels of the estrogen receptor, six electrophilic 11.beta.-Et (C2), 11.beta.-Bu (C4), or 11.beta.-decyl (C10) derivs. of estradiol bearing 11.beta.-terminal electrophilic functionalities, i.e. bromine (C4), (methylsulfonyl)oxy (C2 and C4), bromoacetamido (C2 and C4), and (p-tolylsulfonyl)oxy (C10) were synthesized. The range of their affinity consts. for binding the estrogen receptor was 0.4-37% that of estradiol; the order of increasing affinity (i) relative to the 11.beta.-alkyl arm was Et < Bu and (ii) relative to the electrophilic functionalities was bromoacetamido < bromine < (methylsulfonyl)oxy. Regardless of the conditions used, including prolonged exposure of the receptor to various pH levels (7-9) and temps. (0-25.degree.), the extent of receptor affinity labeling by the 11.beta.-Et and 11.beta.-Bu compds., if any, was under 10%. This was in sharp contrast to results obtained using 11.beta.-((tosyloxy)decyl)estradiol which labeled from 60% to 90% of the receptor hormone-binding sites with an EC50 of .apprx.10 nM. Estrogenic and antiestrogenic activities of the compds. were detd. using the MVLN cell line, which was established from the estrogen-responsive mammary tumor MCF-7 cells by stable transfection of a recombinant estrogen-responsive luciferase gene. The two 11.beta.-Et compds. were mainly estrogenic, whereas the three 11.beta.-Bu and the 11.beta.-decyl compds. essentially showed antiestrogenic activity. The fact that the chem. reactivities of 11.beta.-Et and 11.beta.-Bu compds. were not compromised by interaction with the estrogen receptor made the synthesized high-affinity compds. potential cytotoxic agents which might be able to exert either (i) a specific action on estrogen-regulated genes or (ii) a more general action in estrogen-target cells. Therefore the ability of the compds. (1) to irreversibly abolish estrogen-dependent expression of the luciferase gene and (2) to affect the proliferation of MVLN cells was detd. All electrophiles were able to irreversibly suppress expression of the luciferase gene; the antiestrogenic electrophiles were more potent than the estrogenic ones but less efficient than 4-hydroxytamoxifen, a classical and chem. inert triphenylethylene antiestrogen. Only the antiestrogenic electrophiles decreased cell proliferation; however, they were less potent than 4-hydroxytamoxifen. In conclusion, the synthesized electrophilic estradiol 11.beta.-Et and 11.beta.-Bu derivs. (i) were not efficient affinity labels of the estrogen receptor and (ii) did not display significant cytotoxicity in estrogen-sensitive mammary tumor cells. However, since these derivs. displayed high affinity for the estrogen receptor, they could be used to prep. potential cytotoxic agents which might be selective for tumors affecting estrogen-target tissues, by coupling them with a toxic moiety.

IT **191486-92-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10 carbons

X

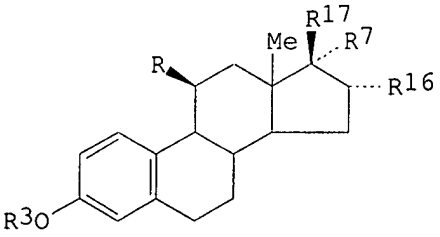
(prepn. of estradiol 11.beta.-n-alkyl derivs. as steroidal affinity labels of the estrogen receptor)

L8 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:31023 HCAPLUS
DOCUMENT NUMBER: 120:31023
TITLE: Preparation of 11.beta.-thiahydrocarbyl-19-norsteroids and analogs as drugs
INVENTOR(S): Claussner, Andre; Nique, Francois; Teutsch, Jean Georges; Van de Velde, Patrick
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9313123 | A1 | 19930708 | WO 1992-FR1193 | 19921217 |
| W: AU, CA, FI, HU, JP, KR, NZ, RU, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| FR 2685332 | A1 | 19930625 | FR 1991-15856 | 19911220 |
| FR 2685332 | B1 | 19950602 | | |
| IL 104105 | A1 | 19970713 | IL 1992-104105 | 19921215 |
| AU 9333570 | A1 | 19930728 | AU 1993-33570 | 19921217 |
| AU 666916 | B2 | 19960229 | | |
| EP 623140 | A1 | 19941109 | EP 1993-902339 | 19921217 |
| EP 623140 | B1 | 19980422 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| HU 68068 | A2 | 19950529 | HU 1994-2134 | 19921217 |
| HU 221482 | B | 20021028 | | |
| AT 165365 | E | 19980515 | AT 1993-902339 | 19921217 |
| RU 2111213 | C1 | 19980520 | RU 1994-31162 | 19921217 |
| ES 2115754 | T3 | 19980701 | ES 1993-902339 | 19921217 |
| ZA 9209859 | A | 19931220 | ZA 1992-9859 | 19921218 |
| CN 1075722 | A | 19930901 | CN 1992-115248 | 19921219 |
| CN 1036718 | B | 19971217 | | |
| US 6281204 | B1 | 20010828 | US 1994-244735 | 19940609 |
| FI 9402944 | A | 19940617 | FI 1994-2944 | 19940617 |
| US 2002072624 | A1 | 20020613 | US 2001-891433 | 20010626 |

PRIORITY APPLN. INFO.: FR 1991-15856 A 19911220
WO 1992-FR1193 A 19921217
US 1994-244735 A3 19940609

OTHER SOURCE(S): MARPAT 120:31023
GI

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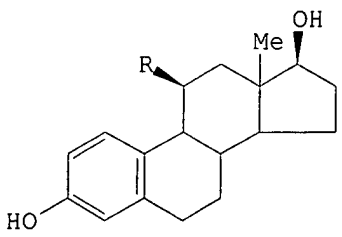



II

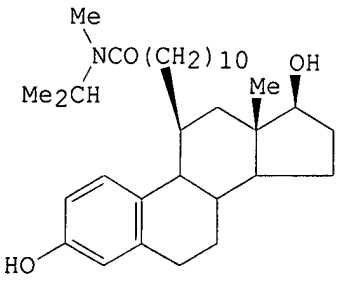
AB Title compds. [I; R = XYSOmZ; R3 = H, (cyclo)alkyl, acyl; R7 = H, alkyl, alkenyl, alkynyl, etc.; R16 = H, halo, alkyl; R17 = OH, CH2OH, acyloxy; R7R17 = O, NOH, NNH2, CH2; X = CH2, arylene(oxy); Y = (O-

interrupted)(satd.) divalent C1-18 aliph. group; Z = (ar)alkyl, aryl; m = 0-2] were prepd. as antiestrogens, antiproliferatives, etc. Thus, 11.beta.-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was condensed with Cl(CH2)5Br and the product converted in 3 steps to estratrienediol II [R = C6H4[O(CH2)5Cl]-4] which was condensed with 2-pyridylmethanethiol to give, after oxidn., II [R = C6H4[O(CH2)5SOZ]-4, Z = 2-pyridylmethyl]. The latter had relative binding affinity (definition given) of 21.2 at mouse estrogen receptors in vitro.

IT **151556-15-9P 151556-16-0P 151556-41-1P 151556-42-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of antiestrogen and antiproliferative)

IT **151555-16-7P 151555-25-8P 151555-26-9P 151555-27-0P 151555-28-1P 151555-54-3P 151555-65-6P 151555-76-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antiestrogen and antiproliferative)

L8 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:401107 HCAPLUS
DOCUMENT NUMBER: 117:1107
TITLE: 11.beta.-Amidoalkyl estradiols, a new series of pure antiestrogens
AUTHOR(S): Claussner, A.; Nedelec, L.; Nique, F.; Philibert, D.; Teutsch, G.; Van de Velde, P.
CORPORATE SOURCE: Cent. Rech., Roussel UCLAF, Romainville, 93230, Fr.
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1992), 41(3-8), 609-14
CODEN: JSBBEZ; ISSN: 0960-0760
DOCUMENT TYPE: Journal
LANGUAGE: English
GI




I

AB In order to find new antiestrogens, devoid of any agonistic activity, a series of 11.beta.-amidoalkyl estradiols were prepd. These compds. were studied in comparison with tamoxifen (TAM): in vitro, for their relative binding affinities (RBA) for mouse and MCF-7 estrogen receptors (ER) and for their antiproliferative effect on MCF-7 (estradiol or EGF/PDGF stimulated) and Ly2 human breast cancer cell lines; in vivo, for their uterotropic/antiuterotropic activities in the mouse and for their antitumoral activities on MCF-7 tumors implanted in nude mice. The most representative compds. are N-methyl-N-isopropyl-(3,17.beta.-dihydroxy-estra-1,3,5(10)-trien-11.beta.-yl)-undecanamide (RU 51625) (I) and its 17.alpha.-ethynyl deriv. (RU 53637). They showed good RBAs for ER and a stronger antiproliferative effect than TAM in vitro. Unlike TAM, these compds. inhibited growth factor-stimulated MCF-7 proliferation, and the growth of the TAM-resistant cell line Ly2. In vivo, they were completely

devoid of uterotropic activity, when given s.c. in mice, but exhibited a slight agonistic effect when administered orally. They showed interesting antitumor activities in nude mice by the percutaneous route, but RU 53637 was more potent than RU 51625 when given orally.

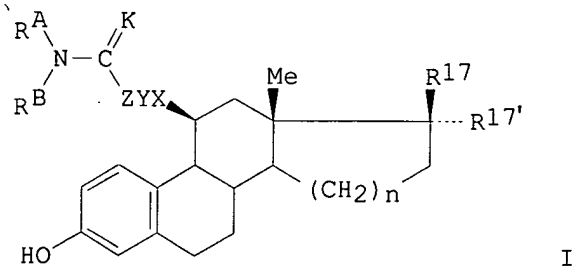
IT **134411-55-5P**, RU 51625 **134411-57-7P**, RU 53637
**134411-74-8P**, RU 50667 **134413-30-2P**, RU 54485
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antiestrogen and antitumor activity of)

L8 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:214774 HCAPLUS
DOCUMENT NUMBER: 116:214774
TITLE: 19-Norsteroids having an amide-bearing chain in the 11-beta position, their preparation, their use as medicines (especially antiestrogens), and pharmaceutical compositions thereof
INVENTOR(S): Claussner, Andre; Nique, Francois; Teutsch, Jean Georges; Van de Velde, Patrick
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Eur. Pat. Appl., 63 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 471612 | A2 | 19920219 | EP 1991-402214 | 19910809 |
| EP 471612 | A3 | 19920513 | | |
| EP 471612 | B1 | 19980128 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| FR 2665901 | A2 | 19920221 | FR 1990-10323 | 19900814 |
| FR 2665901 | B2 | 19940729 | | |
| AT 162797 | E | 19980215 | AT 1991-402214 | 19910809 |
| ES 2112268 | T3 | 19980401 | ES 1991-402214 | 19910809 |
| CA 2049102 | AA | 19920215 | CA 1991-2049102 | 19910813 |
| HU 59416 | A2 | 19920528 | HU 1991-2690 | 19910813 |
| JP 06340688 | A2 | 19941213 | JP 1991-226410 | 19910813 |
| JP 3073803 | B2 | 20000807 | | |
| AU 9182422 | A1 | 19920220 | AU 1991-82422 | 19910814 |
| AU 644671 | B2 | 19931216 | | |
| ZA 9106420 | A | 19921028 | ZA 1991-6420 | 19910814 |
| US 5707982 | A | 19980113 | US 1993-68735 | 19930528 |

PRIORITY APPLN. INFO.:
FR 1990-10323 A 19900814
FR 1989-2384 A 19890224
US 1990-484424 A2 19900223
US 1991-745289 B1 19910814

OTHER SOURCE(S): MARPAT 116:214774
GI



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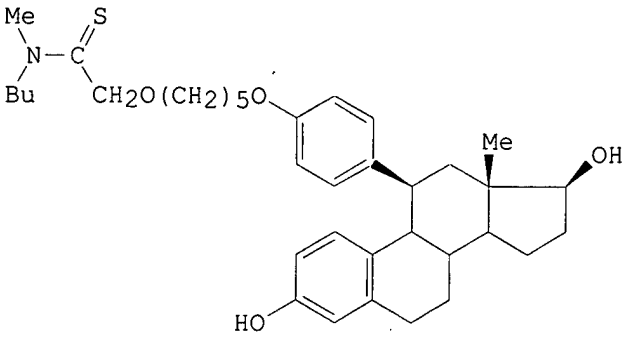


II

AB Twenty title steroids I [either (1) n = 1; K = O; R17 = OH, O2C(CH2)2CO2H or salts; R17' = H, C.tplbond.CH; RA = Me; RB = iso-Pr, Bu, heptafluorobutyl; X = CH2, C6H4, OC6H4; Y = (CH2)7, (CH2)8, (CH2)5C.tplbond.C, (CH2)qOCH2 with q = 5-7, (CH2)5S(O)pCH2 with p = 0-2; Z = bond; or (2) n = 1 or 2; K = O, S; R17 = OH, acyloxy; R17' = H, (substituted) alkyl, alkenyl, or alkynyl; or R17R17' = keto; X = CH2, arylene, OCH2, oxyarylene, thioarylene (bound to steroid at C atom); Y = aliph. chain optionally unsatd. or interrupted by arylene, O, S, SO, or SO2; Z = bond; RA, RB = H, (substituted) alkyl; or RARB = atoms to form (substituted) heterocycle; addnl. restrictions] were prepd. as antiestrogens for treatment of hormone-dependent tumors. For example, 11.beta.-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was etherified with BuNMeCOCH2O(CH2)5Br (prepns. given), followed by isomerization to a 3-hydroxyestra-1,3,5(10)-triene, redn. of the 17-oxo group to 17.beta.-OH with NaBH4, protection of the OH groups as acetates, conversion of the amide to a thioamide with Lawesson's reagent, and deprotection, to give title compd. II. The IC50 of II for inhibiting growth of MCF-7 mammary tumor cells in vitro was 0.03 nM. A tablet formulation comprising I is given.

IT **140712-19-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antiestrogenic antitumor agent)

L8 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:656464 HCAPLUS
DOCUMENT NUMBER: 115:256464
TITLE: Preparation of 19-norsteroids containing an amide or a carboxamide group as drugs
INVENTOR(S): Claussner, Andre; Nedelec, Lucien; Philibert, Daniel; Van de Velde, Patrick
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Eur. Pat. Appl., 128 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 384842 | A1 | 19900829 | EP 1990-400493 | 19900222 |
| EP 384842 | B1 | 19931229 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL | | | | |
| FR 2643638 | A1 | 19900831 | FR 1989-2384 | 19890224 |
| FR 2643638 | B1 | 19910614 | | |
| HU 55032 | A2 | 19910429 | HU 1990-273 | 19900125 |
| HU 207341 | B | 19930329 | | |
| ZA 9001356 | A | 19910424 | ZA 1990-1356 | 19900222 |
| AT 99320 | E | 19940115 | AT 1990-400493 | 19900222 |
| ES 2062431 | T3 | 19941216 | ES 1990-400493 | 19900222 |
| CA 2010826 | AA | 19900824 | CA 1990-2010826 | 19900223 |
| AU 9050072 | A1 | 19900830 | AU 1990-50072 | 19900223 |
| AU 631853 | B2 | 19921210 | | |
| JP 02268194 | A2 | 19901101 | JP 1990-41383 | 19900223 |
| JP 3009169 | B2 | 20000214 | | |
| US 5149696 | A | 19920922 | US 1990-484424 | 19900223 |
| PL 162151 | B1 | 19930930 | PL 1990-283941 | 19900223 |
| CN 1046166 | A | 19901017 | CN 1990-101580 | 19900224 |
| US 5290771 | A | 19940301 | US 1992-875460 | 19920429 |
| US 5707982 | A | 19980113 | US 1993-68735 | 19930528 |

PRIORITY APPLN. INFO.: FR 1989-2384 A 19890224
EP 1990-400493 A 19900222
US 1990-484424 A3 19900223
FR 1990-10323 A 19900814
US 1991-745289 B1 19910814

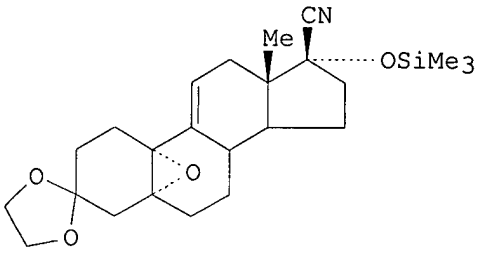
OTHER SOURCE(S): CASREACT 115:256464; MARPAT 115:256464
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

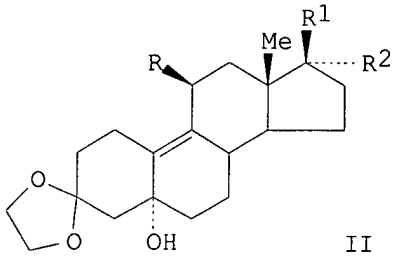
AB The title compds. [I; R, R1 = H, (substituted) alkyl; or NRR1 = (substituted) heterocyclyl; R2 = OH, acyloxy; R3 = H, (substituted) alkyl, alkenyl, alkynyl; or R2R3 = O; X = CH2, arylene, CH2O, aryleneoxy linked to the steroid moiety by C; Y = bond, (substituted) aliph. chain; Z = bond, CH2O linked to Y by C; rings A and B may be (2-substituted) Q, Q1; R4 = H, alkyl], having affinities for receptors of hormones, e.g., estrogen, androgen, progesterone, and therefore useful as inhibitors of hormone-dependent tumors and many other ailments, were prepd. Estradienone II [R5 = OH] [prepd. in several steps from epoxyestrenedione III and p-Me3CSiMe2O(CH2)8C6H4Br] was amidated with HNMeBu to give II (R5 = NMeBu), which was enol-esterified with AcBr and the product hydrolyzed to give I [R = Me, R1 = Bu, X = C6H4, Y = (CH2)7, Z = bond, R2 = OH, rings A and B = Q1, R3 = R4 = H]. This had an IC50 of 0.04 .mu.M against the growth of mammary tumor cells.

IT **134411-55-5P 134411-56-6P 134411-57-7P**
**134411-58-8P 134411-61-3P 134411-65-7P**
**134411-66-8P 134411-67-9P 134411-68-0P**
**134411-71-5P 134411-73-7P 134411-74-8P**
**134411-77-1P 134411-78-2P 134411-81-7P**
**134411-83-9P 134413-12-0P 134413-14-2P**
**134413-15-3P 134413-18-6P 134413-19-7P**
**134413-20-0P 134413-22-2P 134413-24-4P**
**134413-25-5P 134413-28-8P 134413-29-9P**
**134413-30-2P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as drug)

L8 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:498135 HCAPLUS
DOCUMENT NUMBER: 95:98135
TITLE: Regio and stereospecific synthesis of 11.beta.-substituted 19-norsteroids. Influence of 11.beta.-substitution on progesterone receptor affinity - (1)
AUTHOR(S): Belanger, A.; Philibert, D.; Teutsch, G.
CORPORATE SOURCE: Cent. Rech., Roussel-UCLAF, Romainville, 93230, Fr.
SOURCE: Steroids (1981), 37(4), 361-82
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI




I

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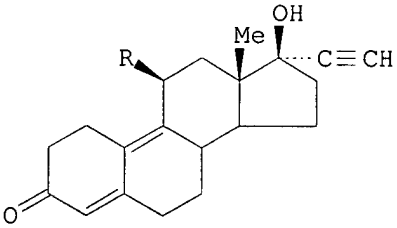


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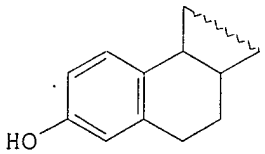


V

AB Epoxyestrene I was treated with R2CuLi (R = alkyl, aryl) or RMgX (X = halo)-CuCl to give estrenols II (R1 = cyano, R2 = OSiMe3), which was ethynylated to norpregnenynediols II (R1 = OH, R2 = C.tplbond.CH) (III). The concomitant deketalization and dehydration of III gave norpregnadienynols IV, which were aromatized to norpregnatrienynols V. The relative affinities for the progestin and estrogen receptors showed very specific interactions between the progesterone receptor and the unsatd. substituents at C-11 of V.

IT **78793-16-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

=> fil caold
FILE 'CAOLD' ENTERED AT 16:05:32 ON 31 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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=> s l7
L9            0 L7

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=> fil reg
FILE 'REGISTRY' ENTERED AT 16:05:48 ON 31 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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provided by InfoChem.

STRUCTURE FILE UPDATES:   30 MAR 2003  HIGHEST RN 500991-80-0
DICTIONARY FILE UPDATES:  30 MAR 2003  HIGHEST RN 500991-80-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
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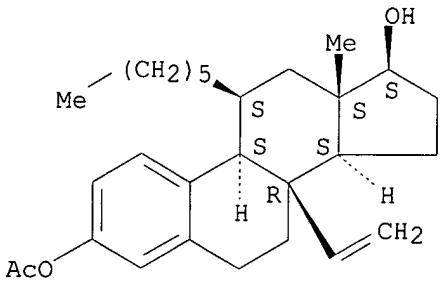
L7 ANSWER 1 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 367269-94-1 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-hexyl-, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
FS STEREOSEARCH
MF C28 H40 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



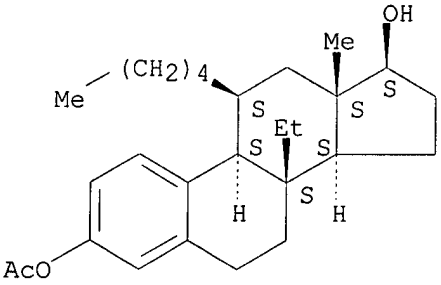

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:318607

L7 ANSWER 5 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 367269-90-7 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
FS STEREOSEARCH
MF C27 H40 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

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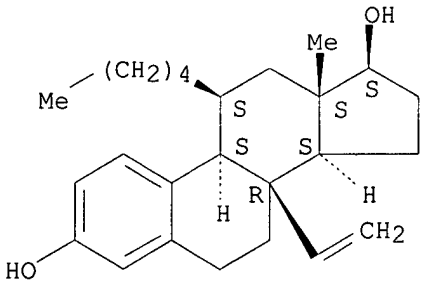
REFERENCE 1: 135:318607

L7 ANSWER 10 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 367269-79-2 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 11.beta.-Pentyl-8.beta.-vinylestra-1,3,5(10)-triene-3,17.beta.-diol
FS STEREOSEARCH
MF C25 H36 O2
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

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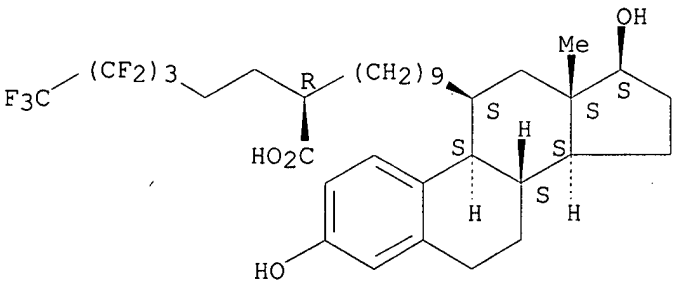
REFERENCE 1: 135:318607

L7 ANSWER 13 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 342899-25-6 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanoic acid, 3,17-dihydroxy-.alpha.-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (.alpha.R,11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H47 F9 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

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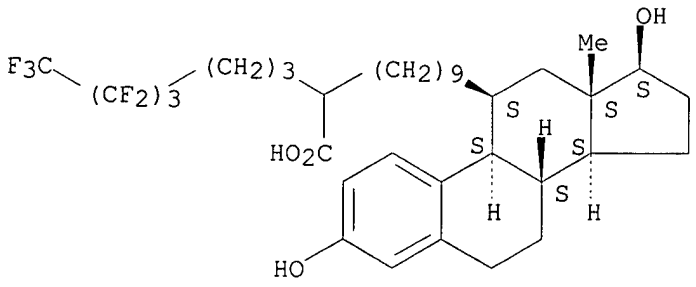
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:19815

L7 ANSWER 15 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 342899-00-7 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanoic acid, 3,17-dihydroxy-.alpha.-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H49 F9 O4

SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



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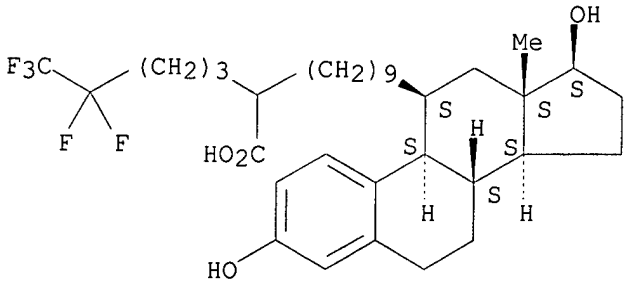
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:19815

L7 ANSWER 16 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 342898-99-1 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanoic acid, 3,17-dihydroxy-.alpha.-(4,4,5,5,5-pentafluoropentyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H49 F5 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



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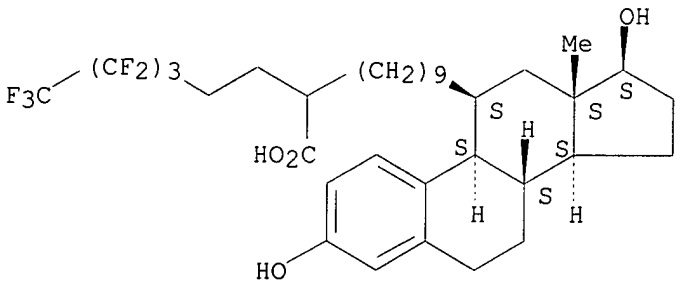
REFERENCE 1: 135:19815

L7 ANSWER 20 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 342898-92-4 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanoic acid, 3,17-dihydroxy-.alpha.-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

MF C35 H47 F9 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



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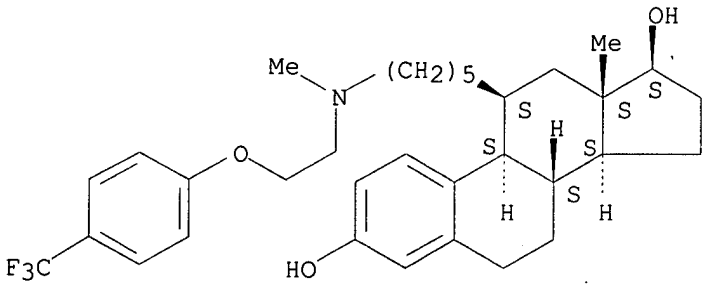
REFERENCE 1: 135:19815

L7 ANSWER 24 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-90-4 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[2-[4-(trifluoromethyl)phenoxy]ethyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H44 F3 N O3
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



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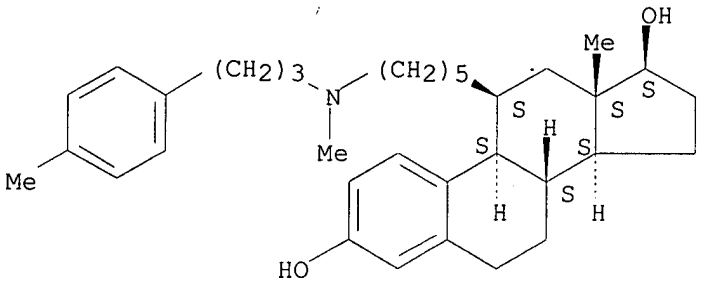
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 30 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-84-6 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-(4-methylphenyl)propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C34 H49 N O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



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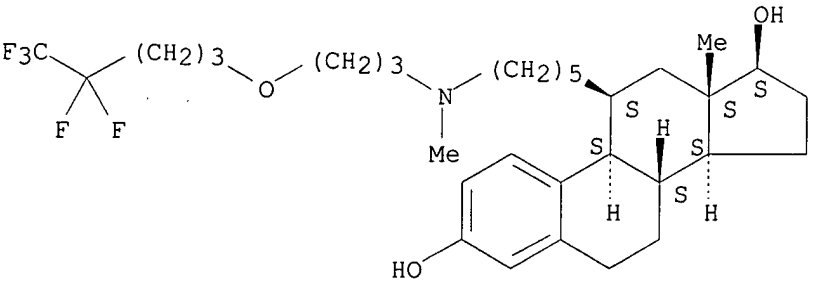
REFERENCE 1: 134:56837

L7 ANSWER 35 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-79-9 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)oxy]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H48 F5 N O3
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



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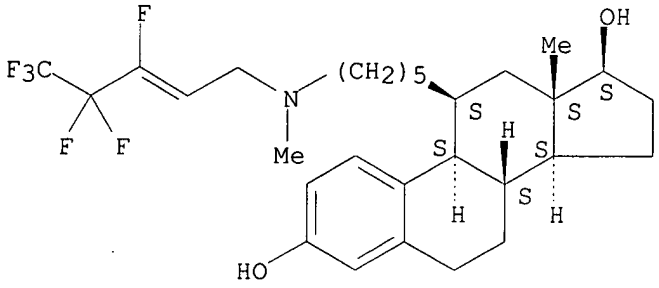
REFERENCE 1: 134:56837

L7 ANSWER 40 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-74-4 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(3,4,4,5,5,5-hexafluoro-2-pentenyl)methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C29 H39 F6 N O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



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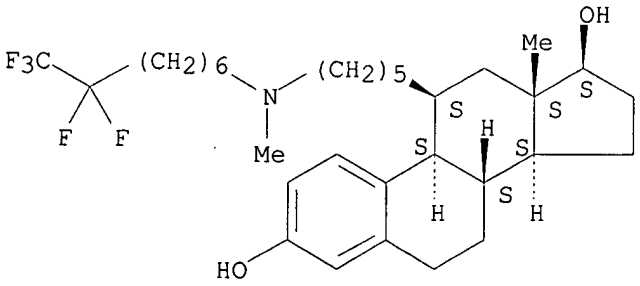
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 45 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-69-7 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(7,7,8,8,8-pentafluorooctyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H48 F5 N O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



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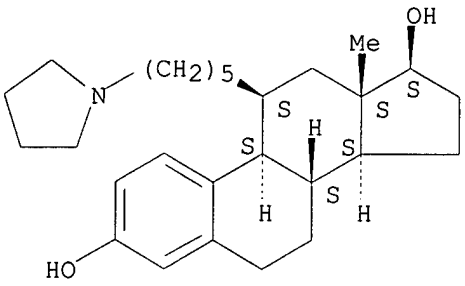
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 50 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-64-2 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-(1-pyrrolidinyl)pentyl]-,

(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H41 N O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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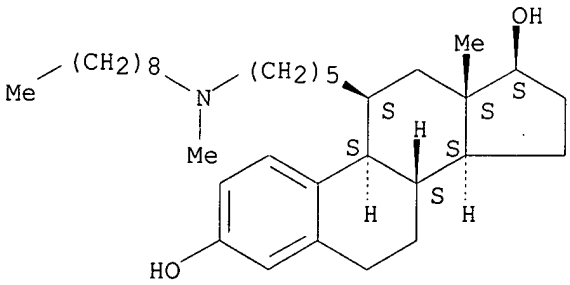
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 55 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-59-5 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-(methylnonylamino)pentyl]-,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H55 N O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

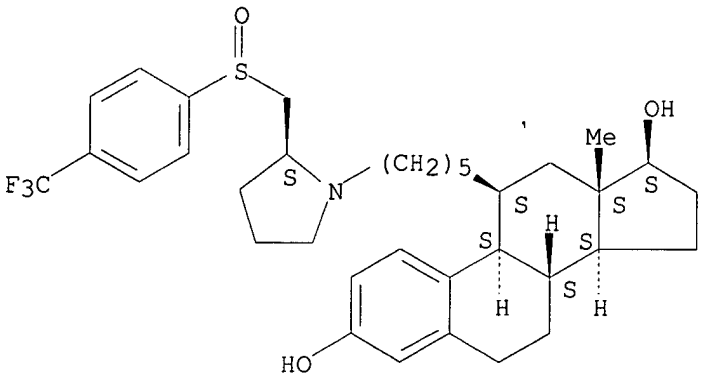
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 60 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-33-5 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(2S)-2-[[[4-
(trifluoromethyl)phenyl]sulfinyl]methyl]-1-pyrrolidinyl]pentyl]-,

(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H46 F3 N O3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



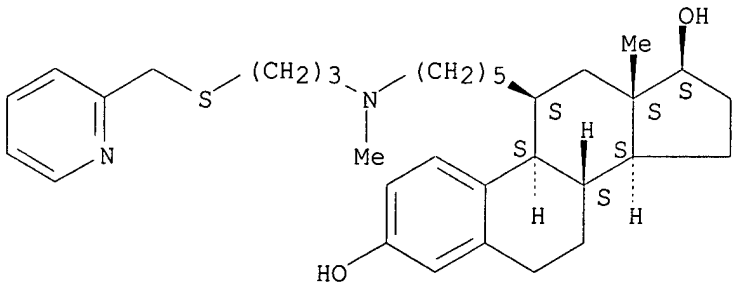
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 65 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 314019-28-8 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[(2-pyridinylmethyl)thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H48 N2 O2 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).



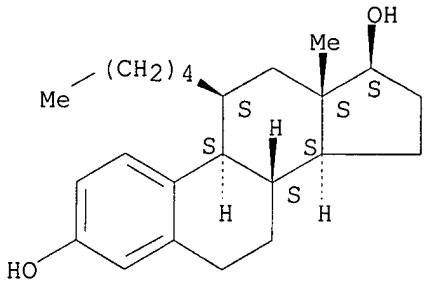
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:56837

L7 ANSWER 68 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 271260-12-9 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-pentyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H34 O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



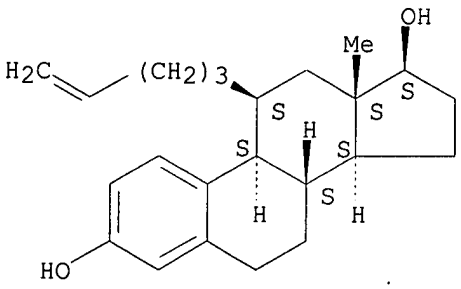

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:4848

L7 ANSWER 70 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 271260-07-2 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-(4-pentenyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H32 O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

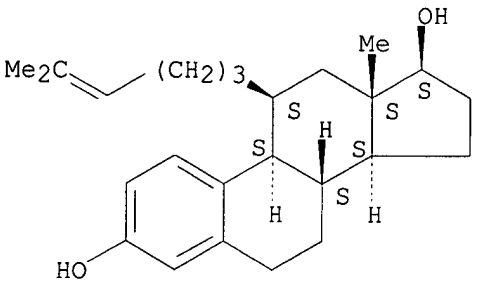
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:4848

L7 ANSWER 72 OF 115 REGISTRY COPYRIGHT 2003 ACS

RN 271259-96-2 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-(5-methyl-4-hexenyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H36 O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



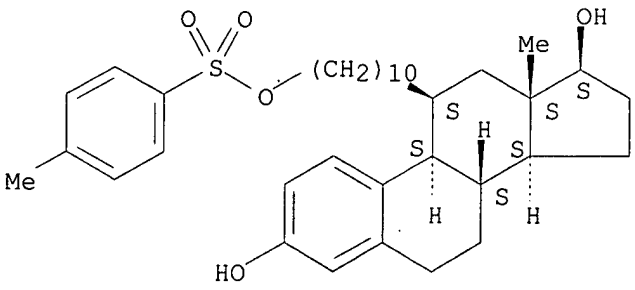

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:4848

L7 ANSWER 73 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 191486-92-7 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[10-[[(4-methylphenyl)sulfonyl]oxy]decyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H50 O5 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

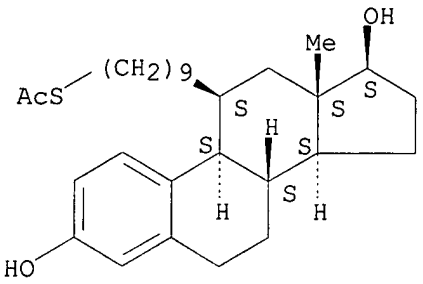
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 127:76140

L7 ANSWER 74 OF 115 REGISTRY COPYRIGHT 2003 ACS

RN 151556-42-2 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[9-(acetylthio)nonyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H44 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



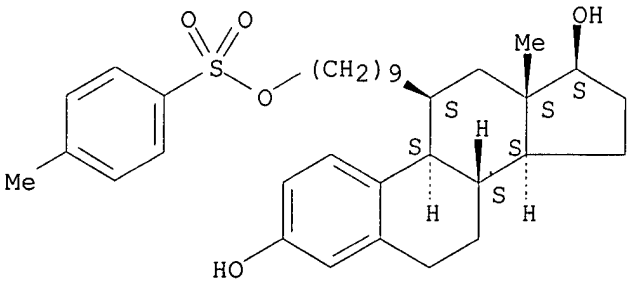

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:31023

L7 ANSWER 75 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 151556-41-1 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[9-[[(4-methylphenyl)sulfonyl]oxy]nonyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H48 O5 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

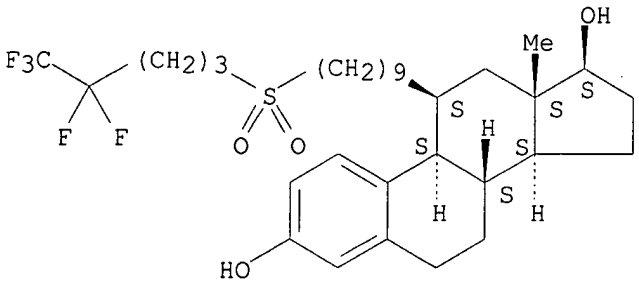
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:31023

L7 ANSWER 78 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 151555-76-9 REGISTRY

CN Estra-1,3,5(10)-triene-3,17-diol, 11-[9-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]nonyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H47 F5 O4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



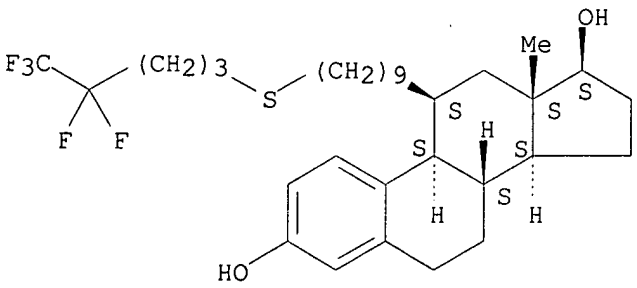
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:31023

L7 ANSWER 80 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 151555-54-3 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H47 F5 O2 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

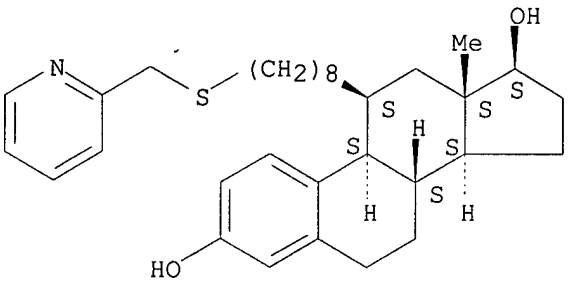
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:31023

L7 ANSWER 85 OF 115 REGISTRY COPYRIGHT 2003 ACS

RN 151555-16-7 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[8-[(2-pyridinylmethyl)thio]octyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H45 N O2 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



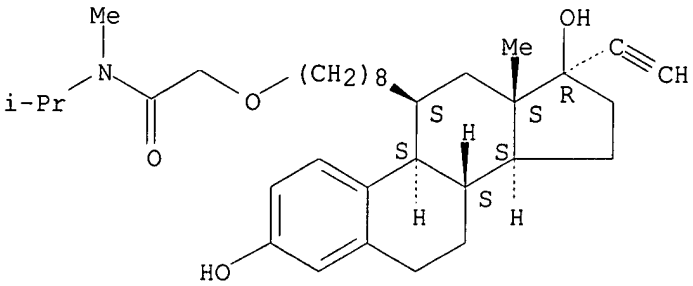

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:31023

L7 ANSWER 86 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 140712-19-2 REGISTRY
CN Acetamide, 2-[[8-[(11.beta.,17.alpha.)-3,17-dihydroxy-19-norpregna-1,3,5(10)-trien-20-yn-11-yl]octyl]oxy]-N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norpregnane, acetamide deriv.
FS STEREOSEARCH
MF C34 H51 N O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



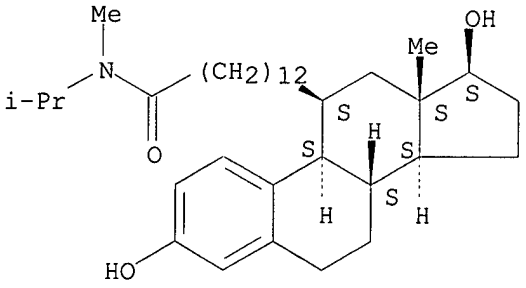

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 116:214774

L7 ANSWER 87 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134413-30-2 REGISTRY
CN Estra-1,3,5(10)-triene-11-tridecanamide, 3,17-dihydroxy-N-methyl-N-(1-methylethyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN RU 54485
FS STEREOSEARCH
MF C35 H57 N O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

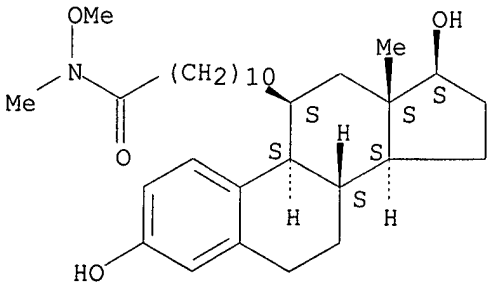
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 117:1107

REFERENCE 2: 115:256464

L7 ANSWER 90 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134413-25-5 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanamide, 3,17-dihydroxy-N-methoxy-N-methyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H49 N O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

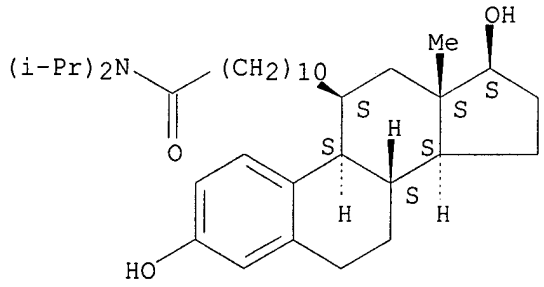
1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 115:256464

L7 ANSWER 95 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134413-18-6 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanamide, 3,17-dihydroxy-N,N-bis(1-methylethyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H57 N O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



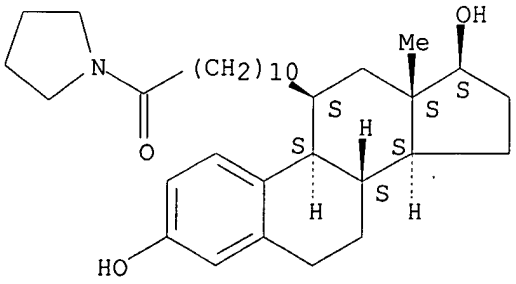

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 115:256464

L7 ANSWER 99 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134411-83-9 REGISTRY
CN Pyrrolidine, 1-[11-[(11.beta.,17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-11-yl]-1-oxoundecyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estrane, pyrrolidine deriv.
FS STEREOSEARCH
MF C33 H51 N O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



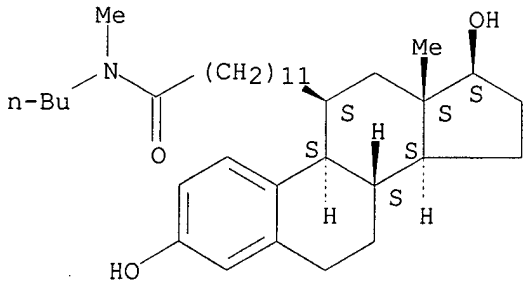

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 115:256464

L7 ANSWER 100 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134411-81-7 REGISTRY
CN Estra-1,3,5(10)-triene-11-dodecanamide, N-butyl-3,17-dihydroxy-N-methyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H57 N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.



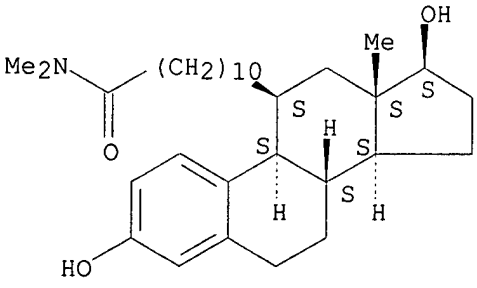

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 115:256464

L7 ANSWER 105 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134411-71-5 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanamide, 3,17-dihydroxy-N,N-dimethyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H49 N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

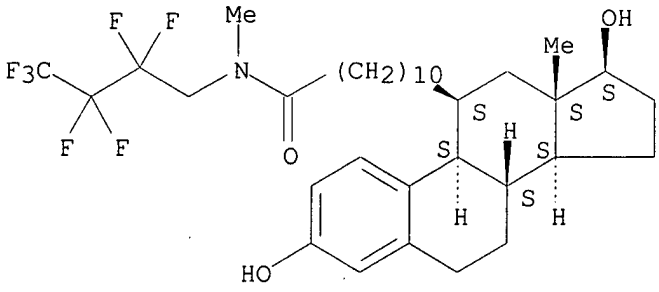
1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 115:256464

L7 ANSWER 110 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 134411-61-3 REGISTRY
CN Estra-1,3,5(10)-triene-11-undecanamide, N-(2,2,3,3,4,4,4-heptafluorobutyl)-3,17-dihydroxy-N-methyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H48 F7 N O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



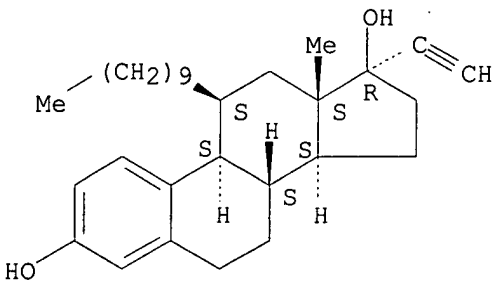
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 115:256464

L7 ANSWER 115 OF 115 REGISTRY COPYRIGHT 2003 ACS
RN 78793-16-5 REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, 11-decyl-, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H44 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 95:98135